

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.46e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.22e-01

Confidence level: 4.66e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethiozin</div> <div>Measured: 2.25e-11</div> <div>Predicted: 4.34e-06</div>	<div>Image not found</div> <div>Coumatetralyl</div> <div>Measured: 6.00e-11</div> <div>Predicted: 2.11e-10</div>	<div>Image not found</div> <div>Butanedinitrile, ethyl-</div> <div>Measured: 3.70e-09</div> <div>Predicted: 1.62e-02</div>
<div>Image not found</div> <div>Ametryn</div> <div>Measured: 2.85e-07</div> <div>Predicted: 1.70e-06</div>	<div>Image not found</div> <div>Niclosamide</div> <div>Measured: 1.49e-11</div> <div>Predicted: 2.02e-11</div>	